Studies of thermal conductivity in FPU-like lattices

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The pioneering computer simulations of the energy relaxation mechanisms performed by Fermi, Pasta and Ulam can be considered as the first attempt of understanding energy relaxation and thus heat conduction in lattices of nonlinear oscillators. In this paper we describe the most recent achievements about the divergence of heat conductivity with the system size in 1d and 2d FPU-like lattices. The anomalous behavior is particularly evident at low energies, where it is enhanced by the quasi-harmonic character of the lattice dynamics. Remakably, anomalies persist also in the strongly chaotic region where long–time tails develop in the current autocorrelation function. A modal analysis of the 1d case is also presented in order to gain further insight about the role played by boundary conditions.

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Almost one century ago Pierre Debjie conjectured that nonlinearities should be considered as a basic ingredient for explaining relaxation and transport mechanisms exhibited by real solids. In fact, the simplest model – a lattice of harmonic oscillators – yields quite an unphysical scenario: any initial excitation does not evolve towards an equilibrium state, but frequently returns close the initial state, while transport is purely ballistic since any Fourier component transfers energy unaltered through the lattice at the sound velocity. In the thirties the introduction of nonlinear terms in a perturbative quantum–mechanical description, allowed Rudolph Peierls to obtain a successful explanation of the thermodynamics of solids at very low–temperature. Only twenty years later Enrico Fermi, John Pasta and Stanley Ulam tackled the problem of studying the relaxation and transport properties of a lattice of nonlinear classical oscillators. As discussed all over this issue, their numerical studies have provided inspiration for an astonishingly large amount of investigations. In this contribution we aim at surveying the progresses and the still open problems concerning heat conduction in the FPU model. In particular, we discuss the divergence of heat conductivity with the system size in the 1d and 2d versions of the model.

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I. INTRODUCTION

At the beginning of the 50's one of the first digital computers, MANIAC 1, was available at Los Alamos National Laboratories in the US. It had been designed by the mathematician J. von Neumann for supporting investigations in several research fields, where difficult mathematical problems could not be tackled by rigorous proofs [1]. Very soon Enrico Fermi realized the great potential of this revolutionary computational tool for approaching also some basic physical questions that had remained open for decades. In particular, MANIAC 1 appeared as a suitable instrument for analyzing the many aspects of nonlinear problems that could not allow for standard perturbative methods. In collaboration with the mathematician S. Ulam and the physicist J. Pasta, Fermi proposed to integrate by MANIAC 1 the dynamical equations of the simplest model of a crystal: a chain of classical oscillators coupled by nonlinear forces described by the Hamiltonian

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + V(q_{i+1} - q_i) \right] \tag{1}$$

where the integer index i labels the oscillators, whose displacements with respect to equilibrium positions and momenta are q_i and p_i, respectively. For the sake of simplicity Fermi, Pasta and Ulam considered the interatomic potentials

$$V(z) = \frac{1}{2} m\omega^2 z^2 + \frac{\alpha}{3} z^3 \tag{2}$$

and

$$V(z) = \frac{1}{2} m\omega^2 z^2 + \frac{\beta}{4} z^4 \tag{3}$$

which have been therafter termed "α" and "β" models respectively. The corresponding equations of motion were implemented by M. Tsingou into a program containing an integration algorithm that MANIAC 1 could efficiently compute.

As discussed elsewhere in this Focus Issue, the FPU numerical experiment was intended to test how equilibrium (equipartition) is approached by an isolated set of nonlinearly coupled oscillators. On the other hand, the connection of this problem to the one of transmission of vibrational energy must not have been escaped to Fermi's physical intuition. Already in 1914, the dutch physicist P. Debye had argued that nonlinearity in the interatomic forces is necessary for the finiteness of thermal conductivity of insulating crystals, i.e. for the Fourier's law $\vec{J} = -\kappa \nabla T$ to hold. Since, despite the many simplifications, this basic ingredient is included in the FPU model, one could hope to describe this important physical effect in a concrete case.

Furthermore, the measurement of the time scale for approaching the equilibrium state, i.e. the"relaxation time" of plane-wave excitations, would have provided an indirect determination of thermal conductivity. Indeed, the most elementary picture of heat conductivity is based on the analogy with kinetic theory of gases where $\kappa = C v_s \ell/3$, C being the heat capacity, v_s the sound velocity and ℓ the mean free path. In a lattice, heat carriers are phonons (classically the normal modes), and it is necessary to take into account that the latter have different group velocities, $v_{\mathbf{k}} = \partial\omega/\partial\mathbf{k}$, depending on their wavenumber $\mathbf{k}$. Accordingly, the above expression for κ generalizes to

$$\kappa \propto \sum_{\mathbf{k}} C_{\mathbf{k}} v_{\mathbf{k}}^2 \tau_{\mathbf{k}} \quad , \tag{4}$$

where we have introduced the relaxation time $\tau_{\mathbf{k}} = \ell_{\mathbf{k}}/v_{\mathbf{k}}$ that can be determined by phenomenologically including all possible scattering mechanisms (anharmonicity, impurities, boundary effects, electrons etc.) that must be determined in some independent way.

In their numerical experiment [2] FPU observed that, at variance with the original intuition, the energy initially fed in one of the low, i.e. long–wavelength, oscillatory mode did not flow to the higher modes, but was exchanged only among a small number of low modes, before flowing back almost exactly to the initial state, yielding a recurrent behavior. Despite nonlinearities were at work, neither a tendency towards thermalization, nor a mixing rate of the energy could be identified. The dynamics exhibited regular features very close to those of an integrable system. Thus, in the spirit of the Debye argument, this infinite relaxation time would imply an infinite conductivity also in presence of nonlinear forces!

This indirect consequence of Fermi, Pasta and Ulam's work received an intuitively appealing confirmation with the discovery of Zabusky and Kruskal's soliton. Generally speaking, whenever the equilibrium dynamics of a lattice can be decomposed into that of independent "modes", the system is expected to behave as an ideal conductor. Besides the trivial example of the harmonic crystal, this applies also to the broader case of integrable nonlinear models characterized by the presence of "mathematical solitons" originating the balance of dispersion and nonlinearity. The idea that solitons may play a role in heat conduction dates back to Toda [3] and has been invoked to explain the anomalous behavior of the FPU model as a consequence of ballistic transport due to solitons of the modified Korteweg–deVries equation (see e.g. [4]). Thereby, the existence of stable nonlinear excitations in integrable systems is expected to lead to ballistic rather than to diffusive transport. As pointed out in Ref. [3], solitons travel freely, no temperature gradient can be maintained and the conductivity is thus infinite.

II. THE NONEQUILIBRIUM FPU MODEL: EARLY RESULTS

The original FPU simulation probed the nonequilibrium transient dynamics under the only effect of internal forces. When dealing with systems that can exchange energy with external reservoirs, one wishes to introduce the effect of external temperature gradients by means of nonequilibrium simulations too. In the spirit of linear response, the two concepts should be to some extent related, since the relaxation of spontaneous fluctuations rules the system response.

In the present context, the natural way to proceed consists in putting the system in contact with two heat reservoirs operating at different temperatures T_+ and T_-. Several methods have been proposed based on both deterministic and stochastic algorithms[5]. Regardless of the actual thermostatting scheme, after a transient, an off-equilibrium stationary state sets in, with a net heat current flowing through the lattice. The thermal conductivity of the chain κ is then estimated as the ratio between the time–averaged flux $\overline{J}$ and the overall temperature gradient $(T_+ - T_-)/L$. Notice that, by this latter choice, κ amounts to an effective transport coefficient including both boundary and bulk scattering mechanisms. The average $\overline{J}$ can be estimated in several equivalent ways, depending on the employed thermostatting scheme. One possibility is to directly measure the energy exchanges with the two baths. A more general definition (thermostat-independent) consists in averaging

$$J = \frac{a}{2} \sum_n (\dot{q}_{n+1} + \dot{q}_n) F_n \quad , \tag{5}$$

that is a suitable microscopic expression appropriate in the context of lattices with nearest–neighbour couplings [6]. Here, $F_n = -V'(q_{n+1} - q_n)$ is a shorthand notation for the force excerted by the n–th on the $n+1$–th oscillator, while a is the lattice spacing.

Historically, this approach has been followed some years after the implications of the original FPU experiment were appreciated by the nonlinear physics commu-

nity. The first papers on the FPU model under steady nonequilibrium conditions date back to the pioneering studies of Payton, Rich and Visscher [9] and Jackson, Pasta and Waters [10]. In both cases, the Authors considered cubic plus quartic potential terms resulting from the expansion of the Lennard-Jones potential. To investigate the effect of impurities in the crystal, either a disordered binary mixture of masses [9] or random nonlinear coupling constants [10] were considered. It should be recognized a posteriori that those very first computer studies attacked the problem from the most difficult side. In fact, even before the effect of disorder was fully understood in harmonic chains, they studied systems where anharmonicity and disorder are simultaneously present. Nevertheless, those early works have the merit to have showed how the interplay of the two ingredients can lead to unexpected results that, in our opinion, are still far from being fully understood. Indeed, Ref.[9] revealed that the simple perturbative picture in which anharmonicity and impurities provide two independent (and thus additive) scattering mechanisms does not hold. More precisely, the Authors found even cases in which anharmonicity *enhances* thermal conductivity. A qualitative explanation was put forward by claiming that anharmonic coupling induces an energy exchange between the localized modes, thus leading to an increase of the heat flux. Additional questions that have been investigated were the effect of disorder on the temperature field and the concentration of impurities. Besides the obvious finding that disorder reduces the value of heat conductivity (for fixed finite-chain length), it was noticed an asymmetric behavior between the case of a few heavy atoms randomly added to an otherwise homogeneous light-atom chain and its converse. The smaller values of the conductivity observed in the former cases were traced back to the larger number of localized modes [9].

Several studies of lattices under energy fluxes as well as attempts of designing easy-to-simulate models followed these first studies. The reader is referred to Ref. [5] for a more detailed account. Among others it is worth mentioning the example of the so-called ding-a-ling model [11] that was the first example where the validity of the Fourier's law was convincingly shown. Besides this neat instance (that actually belongs to a different class of 1d chains which include the interactions with an external substrate [12]), many (sometimes contradicting) results and interpretations appeared in the literature. In retrospective, these difficulties can be traced back to the presence of very strong correlations and slow dynamics that was unexpected for such simple models and that could not be tackled due to computational limits. In the next sections, we illustrate how and why the Fourier's law breaks down in the 1d FPU model.

III. THE QUASI-INTEGRABLE LIMIT

A remarkable property of models like (1) is the existence of two distinct dynamical regimes for the relaxation dynamics. For the FPU–model, the existence of an *energy threshold* was identified numerically by Bocchieri et al. [13] and confirmed by the resonance–overlap criterion proposed by Chirikov and coworkers [14]. Further numerical experiments (see Ref. [15] and reference therein) showed that there exists a value of the energy density e_c below which almost–regular behavior significantly slows down the relaxation. This originates from the fact that, although primary resonances do not overlap, higher order resonances can do, yielding a slower evolution in phase space on a time scale that is inversely proportional to a power of the energy density [16]. Conversely, above e_c, equipartition is rapidly reached during a typical simulation run. For this reasons, e_c has been termed *strong stochasticity threshold* [17]. Although the above analysis was mainly focused on the FPU–β model, it has been shown that such a threshold generically exists for several lattice models in 1 and 2d [15].

A related finding is the dependence of the maximal Lyapunov exponent λ on the energy density. An analytic estimate of λ for the FPU–β problem has been also provided [18]

$$\lambda(e) \sim \begin{cases} e^2 & \text{for } e < e_c. \\ e^{1/4} & \text{for } e > e_c; \end{cases} \qquad (6)$$

This implies that the "correlation" time due to the presence of chaotic instabilities (i.e. the inverse of λ) may become exceedingly large for small enough values of e.

The existence of long–lasting transients and the fact that the Lyapunov time–scale becomes very large both suggest that also stationary transport properties below e_c may be strongly affected by the quasi–integrability of the dynamics. To investigate this features, we simulated the FPU-β chain in contact with reservoirs at different temperatures. For computational convenience, the parameters m, ω and β have been fixed to unity so that the only relevant physical parameter is the energy per particle e. With this choice the threshold energy is $e_c \simeq 0.1$ [17]. The average temperature $T = (T_+ + T_-)/2$ has been chosen to yield an average internal energy of the chain below e_c. We have used the Nosé–Hoover thermostats described in detail in Ref. [5]. In order to fasten the convergence towards the stationary state, the initial conditions have been generated by thermostatting each particle to yield a linear temperature profile. This method is very efficient, especially for long chains, when bulk thermalization may be significantly slow. Simulations of the FPU–β model with chains of length up to 65536 sites and free boundary conditions exhibit a monotonous increase of the finite–size conductivity (see Fig. 1). The growth is linear at small lengths and crosses over to a slower increase. This is best seen as a systematic decrease of the

effective exponent

$$\alpha_{\rm eff}(N) \;=\; \frac{d\ln\kappa}{d\ln N}, \qquad (7)$$

from $\alpha_{\rm eff} \simeq 1$ to a $\alpha_{\rm eff} \simeq 0.5$ (see Fig. 2).

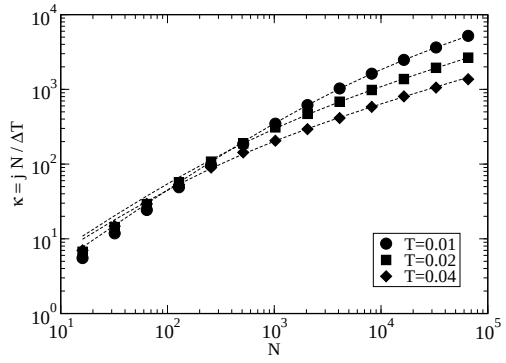

FIG. 1: Finite-size conductivity for the FPU-β model below the strong stochasticity threshold for three different choices of the boundary temperatures $T_\pm = T \pm \Delta T/2$; $\Delta T = 0.01$. Nosè–Hoover thermostat with response times fixed to 0.5; each point results from an average over a single trajectory of about 10^6 time units. Dashed lines are the best fits according to Eq. (8).

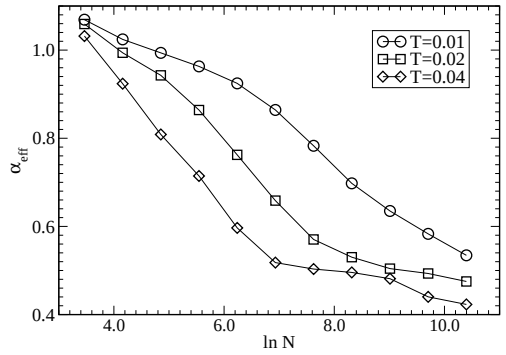

FIG. 2: The effective exponent $\alpha_{\rm eff}$ of the finite-size conductivity for the FPU–β model below the strong stochasticity threshold. Points are obtained by evaluating the centered differences from data in the previous figure.

The data reported in Fig. 1 does not a priori exclude the possibility of a slow convergence to a constant value. Since we rather expect a power law divergence (see next section) we tentatively fitted the conductivity data with a form (see also [19])

$$\frac{1}{\kappa(N)} \;=\; \frac{a}{N} \;+\; \frac{b}{N^\alpha} \qquad (8)$$

The results of the nonlinear fit are shown as solid lines in Fig. 1 and the fitted parameter are reported in Table I. Notice that the exponent α is almost independent of the temperature.

TABLE I: Fitting parameteters, (Eq. 8)

T	a	b	α
0.01	2.00	0.013	0.400
0.02	1.28	0.039	0.423
0.04	1.31	0.059	0.404

Transport properties can be analyzed by computing the power spectrum $S(f)$ of the heat current J at equilibrium. We choose to work in the microcanonical ensemble and integrated the equations of motion with periodic boundary conditions and zero total momentum with a fourth–order symplectic algorithm [20]. The spectra obtained for three different energies roughly corresponding to the average temperatures in Fig. 1 are reported in Fig. 3. By comparing the results obtained for different chain lengths, it is possible to conclude that finite-size corrections are negligible in the considered spectral range. From the inset, where the logarithmic derivative

$$\delta_{\rm eff}(f) \;=\; \frac{d\ln S}{d\ln f} \quad . \qquad (9)$$

is reported versus the frequency f, one can notice that the Lorenzian tail observable at high frequencies starts to cross over towards a regime characterized by a weaker divergence and presumably controlled by the same mechanisms operating in the strong chaotic regime (see next section). Although one can see some evidence of a second plateau only for the largest temperature ($T = 0.04$ – see diamonds in the inset of Fig. 3), it is possible to investigate how the crossover time t_c increases upon decreasing the energy density by suitably rescaling the frequency axis. As a result, it turns out that t_c is roughly proportional to $e^{-1.6}$, which is not too far from the divergence e^{-2} of the Lyapunov time–scale in the weakly chaotic regime (see Eq. (6)). It is thus reasonable to infer that the dynamical mechanisms underlying the slow relaxation and the anomalous conduction are basically the same at such low temperatures.

IV. THE STRONG–CHAOS REGIME

In the previous section we saw how the almost–regular features of the dynamics may give rise to a breakdown of a macroscopic transport law (the Fourier's law in this case). On the basis of the previous discussion, it might be surmised that above the strong stochasticity threshold such anomalies should somehow disappear as the dynamics becomes more "mixing" and the relaxation times shorter. It thus came as a surprise [21] when the anomalous transport features of the FPU chain were actually discovered to persist also in this regime [22]. The origin of this anomalous behavior is twofold. The first cause is the *reduced dimensionality*. Indeed, strong spatial constraints can significantly alter transport properties: the

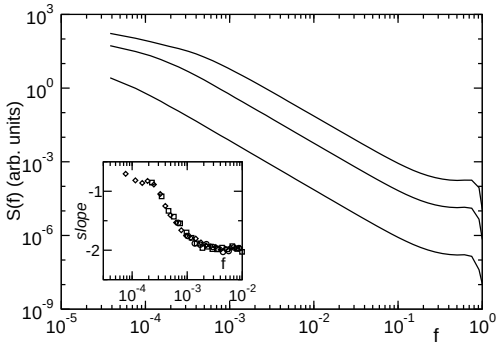

FIG. 3: Power spectra of the flux J as defined in Eq. (5) for the quartic FPU–β model with $N = 2048$ (solid). Data are averaged over about 2500 random initial conditions. To minimize statistical fluctuations, a binning of the data over contiguous frequency intervals has been performed. The curves are for energies $e = 0.01$, $e = 0.02$, $e = 0.04$ (bottom to top) and have been vertically shifted for clarity. In the inset, the logarithmic derivative is reported versus the frequency, after a suitable rescaling of the latter quantity. Circles, squares and diamonds refer to $e = 0.01$, 0.02, and 0.04, respectively.

response to external forces depends on statistical fluctuations which, in turn, crucially depend on the system dimensionality D. This is very much reminiscent of the problem of long–time tails in fluids [23] where, for $D \leq 2$, transport coefficients may *not exist at all*. The second necessary condition is *momentum conservation* i.e. the existence of long-wavelength (Goldstone) modes that are propagating and very weakly damped (τ_k diverges for small k). This latter condition is necessary for these anomalies to occur and means that no external (i.e. substrate) forces must be present. This is precisely the case of the cited ding-a-ling model [11] and of other models in the same class (the nonlinear Klein-Gordon chain for example [12]). The only remarkable exception to this is the coupled rotor chain where, however, different mechanisms are at work [24].

Anomalous behaviour means both a nonintegrable algebraic decay of equilibrium correlations of the heat current $J(t)$ (the Green-Kubo integrand) at large times $t \to \infty$ and a divergence of the finite-size conductivity $\kappa(L)$ in the $L \to \infty$ limit. As a results of a series of simulation studies [5], it can be stated that for 1d lattice models one finds

$$\kappa(L) \propto L^{\alpha} \quad , \qquad \langle J(t)J(0)\rangle \propto t^{-(1+\delta)} \quad , \tag{10}$$

where $\alpha > 0$, $-1 < \delta < 0$, and $\langle\ \rangle$ is the equilibrium average. For small applied gradients, linear-response theory allows establishing a connection between the two exponents. By assuming that $\kappa(L)$ can be estimated by cutting-off the integral in the Green-Kubo formula at the "transit time" L/v (v being some propagation velocity of excitations), one obtains $\kappa \propto L^{-\delta}$ i.e. $\alpha = -\delta$.

It is thus natural to argue about the universality of the exponent α. On the one hand, two independent theoretical approaches, self-consistent mode-coupling approximation [25, 26, 27] and kinetic theory [28], yield $\alpha = 2/5$. On the other hand, a renormalization group calculation on the stochastic hydrodynamic equations for a 1d fluid [29] gives $\alpha = 1/3$. Validation of one of the theories is still under debate, and the existence of crossovers among different scaling regimes has been observed [26]. The available numerical data for α range from 0.25 to 0.44 [5, 30]. As a word of caution, it must be stressed that a numerical estimates are indeed challenging. Even in the most favorable case of computationally efficient models, as the $1D$ gas of hard-point particles with alternating masses [31], finite–size corrections to scaling are sizeable. As a matter of fact, estimates of α as diverse as 0.33 [32, 33] and 0.25 [34] for comparable parameter choices have been reported. Although in this latter instance the anomaly is possibly due to the lack of microscopic chaos [32], it is a generic fact that sensible results require reaching the limits of present computing resources. For instance, in the case of the FPU chain, the best estimate sofar (see below) required simulations of up $\mathcal{O}(10^4)$ particles and $\mathcal{O}(10^8)$ integration steps (plus ensemble averaging) [30].

Since we are interested in the long–wavelength and small–frequency behavior, it is convenient to consider a highly nonlinear model in the hope that the asymptotic regime sets in over shorter time and space scales. Moreover, it is advisable to work with a computationally simple expression of the force. A reasonable compromise is the "infinite temperature" FPU model [30]

$$V(z) \ = \ \frac{1}{4}\, z^4 \quad . \tag{11}$$

This model has no free parameters: since the potential expression is homogeneous, the dynamics is invariant under coordinate rescaling, so that the energy per particle e can be set, without loss of generality, equal to 1.

The power spectra $S(f)$ of J are reported in Fig. 4. The long–time tail (10) corresponds to a power–law divergence f^{δ} in the low-f region. By comparing the results obtained for different numbers of particles, one can clearly see that finite-size corrections are negligible above a size-dependent frequency $f_c(N)$. By fitting the data in the scaling range $[f_c(N), f_s]$, where $f_s \simeq 10^{-3}$, we find $\delta = -0.39(6)$. These values are consistent with previous, less-accurate, findings for similar models, such as the standard FPU [27, 35] and the diatomic Toda [31] chains, thus confirming the expectation that they all belong to the same universality class.

In order to perform a more stringent test of the scaling behavior, we again evaluateid the logarithmic derivative (9) for different frequencies. Since finite-size effects are responsible for the saturation of $S(f)$ when $f \to 0$, $f_c(N)$ can be identified (see Fig. 4) as the frequency below which $\delta_{\rm eff}$ starts growing towards zero. Above f_c, the quality of our numerical data allows revealing a slow but systematic decrease of $\delta_{\rm eff}$ upon decreasing f, which approaches -0.44, a value that is incompatible not only with the renormalization-group prediction of Ref. [29], but also

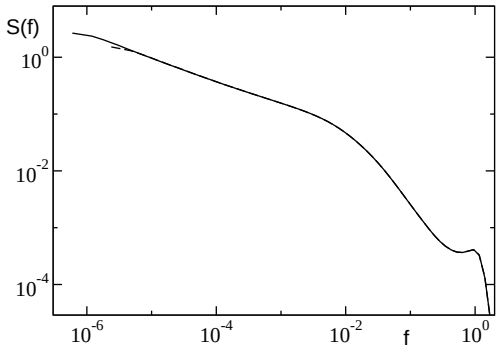

FIG. 4: Power spectra of the flux J as defined in Eq. (5) for the quartic FPU model (11) with $N = 2048$ (solid) and 1024 (dashed). Data are averaged over 30,000 random initial conditions. To minimize statistical fluctuations, a binning of the data over contiguous frequency intervals has been performed.

with the result of mode–coupling [25, 27] and kinetic [28] theories. Furthermore, convergence seems not fully achieved in the accessible frequency range.

To check the consistency of equilibrium and nonequilibrium simulations, one can assume, following the argument exposed below Eq. (10), that the finite–size conductivity $\kappa(L)$ (with $L = Na$) is determined by correlations up to time $\tau = L/v_s$, where v_s is the sound velocity. This means that the frequency f can be turned into a length $L = v_s/f$. It might be argued that the absence of a quadratic term in (11) prevents a straightforward definition of such a velocity in the $T = 0$ limit; nevertheless, it has been shown [36] that an effective phonon dispersion relation at finite energy density can be evaluated for model (11), yielding $v_s = 1.308$ at $e = 1$. Using this value, we can ascertain that, at least for $N > 1000$, there is an excellent agreement between the two approaches (see again Fig. 5).

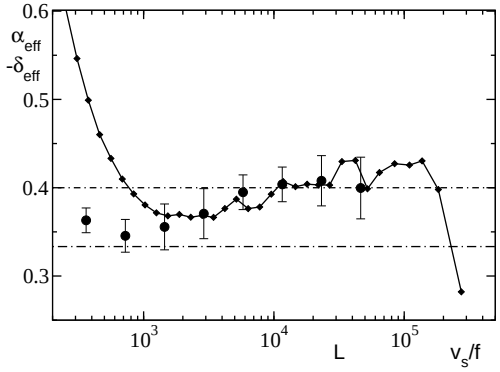

FIG. 5: Quartic FPU model: the effective exponent $\alpha_{\rm eff}$ of the finite-size conductivity for $T_+ = 1.2, T_- = 0.8$ (full dots), compared with the results ($-\delta_{\rm eff}$) of equilibrium simulations. The two horizontal lines correspond to the theoretical predictions, 1/3 and 2/5.

Another way to detect hydrodynamic anomalies is to measure the equilibrium structure factors, namely the averaged power spectra of the mode amplitudes

$$Q_k \;=\; \frac{1}{\sqrt{N}} \sum_{n=1}^{N} q_n \, e^{-i\frac{2\pi k}{N} n} \qquad (12)$$

The spectra display a phonon–like peak at a frequency which is in excellent agreement with the one computed in Ref. [36] (see Fig. 6): the estimated sound speed is $v_s = 1.34 \pm 0.04$, see above. The peaks' linewidths provide a measure of the inverse of the relaxation times; they are found to scale as a power of the wavenumber (see Fig. 7) with an exponenent which is very close to the estimate 5/3 based on arguments of mode-coupling theory [25]. Notice that in the standard case one would rather expect a quadratic law, corresponding to the usual friction term of elasticity theory.

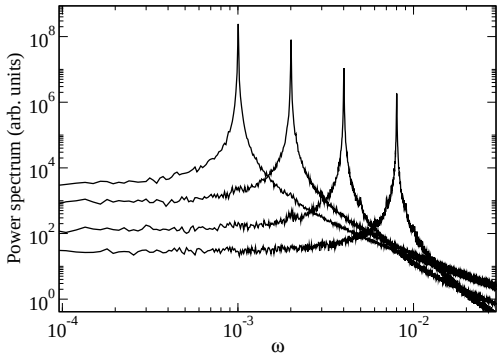

FIG. 6: Structure factors for the quartic FPU model (11) with $N = 8192$ (solid) for the modes of indexes $k = 1, 2, 4, 8$ (left to right). Microcanonical simulations are performed for the energy density $e = 1$ and averaged over an ensemble of about 200 initial conditions.

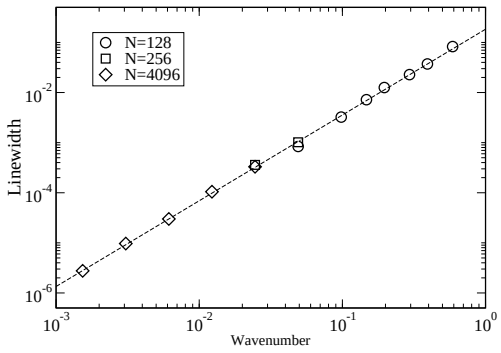

FIG. 7: The wavenumber dependence of the linewidths for the quartic FPU model (11). The linewidths are obtained by fitting the peaks of the spectra for different chain lengths with a lorenzian lineshape. The dashed line is a power–law fit yielding an exponent 1.677 ± 0.025.

V. MODAL ANALYSIS

Conductivity properties are mostly investigated in real space because one is interested in the dependence of the heat flux on the system size. Nevertheless, the renormalization group analysis has teached us that a (spatial) Fourier analysis can be very useful especially to understand anomalous scaling behaviours. Additionally, in the case of integrable systems, a modal analysis allows solving the problem by decomposing it into many independent parts; last but not least the effect of boundary conditions can be better appreciated. In spite of such advantages, very few numerical studies have been devoted to investigating heat conductivity in Fourier space for nonlinear chains [5, 37]. Here in the following, we summarize the current understanding and discuss the open problems with the help of numerical simulations to have some hints about the expected scenario.

As proposed in Ref. [37], it is convenient to start from the formal energy balance

$$J_k^+ + J_k^- + J_k^{nl} = 0, \tag{13}$$

where J_k^+, J_k^-, and J_k^{nl} denote the energy exchanged (per unit time) by the kth mode with the hot, cold heat bath, and with the other modes, respectively. By summing over the index k, one finds that

$$J^+ + J^- = 0, \tag{14}$$

where $J^\pm$ is the total energy flowing from (to) the hot (cold) bath; in fact $\sum_k J_k^{nl} = 0$, since the energy of the system is, on the average, constant. As a result, the total heat flux J can be, e.g., decomposed in modal contributions,

$$J = \sum_k J_k^+ \tag{15}$$

So far, this is just a formal statement. In order to make it operative, it is necessary to give an explicit definition of the modal fluxes. Using the definition (12), one can show that the dynamics of the kth mode is described by the following equation

$$\ddot{Q}_k + \omega_k^2 Q_k + \phi_k^{nl} + \phi_k^+ + \phi_k^- = 0, \tag{16}$$

where ω_k is the frequency of the k mode (which follows from an energy dependent renormalization of the harmonic frequency), while ϕ_k^{nl} is the effective force due to the interactions with all other modes, while $\phi_k^\pm$ account for the interaction with the thermal baths.

Upon multiplying Eq. (16) by $\dot{Q}_k$, and introducing the modal energy $E_k = (\dot{Q}_k^2 + \omega_k^2 Q_k^2)/2$, it follows that

$$0 = \langle \dot{E}_k \rangle = \langle \phi_k^{nl} \dot{Q}_k \rangle + \langle \phi_k^+ \dot{Q}_k \rangle + \langle \phi_k^- \dot{Q}_k \rangle \tag{17}$$

where $\langle \cdot \rangle$ denotes a time average and the first equality is a trivial consequence of stationarity. Since we are assuming that the lattice spacing is $a = 1$, it is now clear that the three terms in the r.h.s. of the above equations coincide with the modal fluxes J_k^{nl}, J_k^+, and J_k^-, respectively.

All such contributions can be easily computed when the interaction with the thermal bath amounts to instantaneous stochastic collisions occurring to either the first or last particle. In such cases, the fluxes $J_k^\pm$ can be easily computed by a mode expansion of the energy locally exchanged in each collision, while J_k^{nl} can be obtained from the energy variation in between collisions.

In a linear chain, the eigenmodes are independent of each other, so that the term J_k^{nl} vanishes. In such conditions, the effective equation of the kth wavevector reduces to

$$\ddot{Q}_k + \omega_k^2 Q_k + \gamma_k^+ \dot{Q}_k + \gamma_k^- \dot{Q}_k + \xi^+ + \xi^- = 0, \tag{18}$$

where $\gamma_k^\pm$ gauges the interaction with the thermal bath while $\xi_k^\pm$ is a Gaussian white noise, whose diffusion constant is, according to the fluctuation-dissipation theorem, $D_k^\pm = k_B T^\pm \gamma_k$. The above equation is nothing but a Langevin equation describing an "oscillator" with a dissipation $\gamma_k^+ + \gamma_k^-$ and an effective noise corresponding to the intermediate temperature $T = (\gamma_k^+ T^+ + \gamma_k^- T^-)/(\gamma_k^+ + \gamma_k^-)$. Although the average energy of the oscillator neither increases nor decreases, the energy exchanged per unit time with each bath

$$J_k^\pm = -\gamma_k^k \langle \dot{q}_k^2 \rangle - \langle \xi^+ \dot{q}_k^2 \rangle \tag{19}$$

is different from zero.

Let us illustrate this under the simplifying but otherwise general assumption of equal coupling strength with the heat baths ($\gamma_k^+ = \gamma_k^- = \gamma_k$). In fact, in this case, $T = T_a = (T^+ + T^-)/2$ so that the energy exchanged with the hot heat bath is $J_k^+ = -2\gamma_k T + 2\gamma_k T^+ = \gamma_k (T^+ - T^-)$, i.e. $J_k \approx \gamma_k$. Conductivity properties can thus be understood from the coupling strength of the eigennodes. In harmonic systems, it is well known that γ_k is proportional to the square amplitude of the kth eigenmode at the chain end [5]. For fixed and free b.c., $\gamma_k \approx k^2/N^3$, $\gamma_k \approx 1/N$, respectively (for the sake of simplicity, we neglect the nonlinear dependence on k, that is important only at large wavenumbers). Since the total heat flux is obtained by summing all contributions up to $k = N$, it follows that J is a quantity of order one independently of the b.c..

The scenario becomes very different if some disorder is added, because the exponential localization of the eigenmodes makes their coupling with the heat baths basically negligible. In such conditions, only the first $\sqrt{N}$ modes are sufficiently extended to appreciably contribute to the heat flux. For free b.c., the total flux being the sum of the contribution is on the order of $1/\sqrt{N}$ which corresponds to a square root divergence of the condcutivity κ. On the contrary, for fixed b.c., the sum of $\gamma_k = k^2/N^3$ yields $J \approx 1/N^{3/2}$, i.e. a vanishing conductivity. In other words, in the presence of disorder, a change of b.c. may turn a "heat superconductor" into a very good insulator!.

The question then arises of how the scenario modifies in the presence of nonlinearities. Past investigations of the FPU models clearly indicate that in the absence of interactions with thermal baths, the dynamics of a Fourier mode with small k is well described by the Langevin equation [39]

$$\ddot{Q}_k + \omega_k^2 Q_k + \gamma_k^{nl}\dot{Q}_k + \xi^{nl} = 0 \quad . \tag{20}$$

According to mode-coupling theory, $\gamma_k \approx (k/N)^{5/3}$ an estimate that is very close to the numerical values (see also Fig. 7). It thus appear natural to assume that in the presence of heat baths, the above equation modifies to

$$\ddot{Q}_k + \omega_k^2 Q_k + (\gamma_k^{nl} + 2\gamma_k)\dot{Q}_k + \xi^{nl} + \xi^{+} + \xi^{-} \tag{21}$$

although we anticipate that the effective value of the coupling γ_k with the heat bath cannot be the same as in the harmonic case. We start addressing the problem of the effective temperature of the kth mode. By repeating the same arguments that lead to predict a temperature T_a in the harmonic case, we obtain now $T_k = [2\gamma_k T_a + \gamma_k^{nl} T_k^{nl}]/(2\gamma_k + \gamma_k^{nl})$ where we write T_k to emphasize a possible dependence of the temperature on the wavenumber and where T_k^{nl} is basically unknown, and it is expected to range between T^- and T^+. For free b.c., $\gamma_k \approx 1/N$, thus implying that there exists a critical value $k_c \approx N^{2/5}$ below which γ_k^{nl} is negligible with respect to γ_k and viceversa above it. As a result, below k_c, we expect $T_k = T_a$, while above, there should be a crossover towards the unknown value T_k^{nl}. Simulations performed in chains of different lengths with $T^+ = 10$ and $T^- = 8$ are trivially in agreement with this scenario. Indeed, T_k determined by evaluating the kinetic temperature of the kth mode is constantly equal to $T_a = 9$. This implies that in spite of the nonlinearity in the profile, modal temperatures behave exactly as in the harmonic case (and also as when the Fourier law would apply). The same is true also for free boundary conditions when, being $\gamma_k = k^2/N^3$, there does not exist a value k_c, since external dissipations should be always negligible.

Let us now analyse the behaviour of modal fluxes. As the internal noise temperature adjusts itself to the arithmetic average of the heat-bath temperatures, the flux J_k^{nl} should vanish. This is confirmed by our simulations: the small values of J_k^{nl} that we have obtained can indeed be interpreted as statistical fluctuations. Much more intriguing is the analysis of the true energy fluxes $J_k^{\pm}$. With reference to free boundary conditions, the integral flux due to the modes with $k < k_c$ scales as $1/N^{3/5}$ and this would be consistent with the direct computations of heat conductivity, were the contribution of $J_k^{\pm}$ for $k > k_c$ negligible. Unfortunately, if we assume that γ_k keeps scaling as $1/N$ (like in the harmonic case) we are led to conclude that all channels equally contribute to the heat flux with a consequent linear divergence of the conductivity with the system size! We already know that this is not the case, but the data reported in Fig. 8 give us some hints about possible explanations of this failure. In the figure

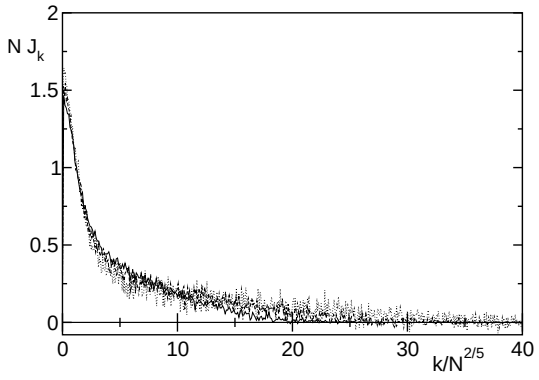

FIG. 8: Modal flux J_n (multiplied by the chain length N versus the scaled wavenumber $k/N^{2/5}$ for an FPU-β lattice with free boundary conditions. The solid, dashed and dotted lines refer to $N = 256$, 512 and 1024, respectively. Averages are taken over a time span of 10^8 units.

we report the modal flux multiplied by N versus $k/N^{2/5}$ for three different chain lengths. The reasonably good overlap confirms the hyphotesis that for $k < k_c \approx N^{2/5}$, the internal dissipation is negligible and the system behaves like a harmonic chain. On the other hand, the decrease of J_k suggests that above k_c the effective coupling with the thermal baths is much smaller than $1/N$. Determining the dependence of γ_k on k in this regime is, to our knowledge, an open problem. Solving this problem is all the way more crucial in the context of fixed boundary conditions where γ_k must differ everywhere from the harmonic chains. In fact, simulations publised elsewhere [5] indicate that, at variance with the harmonic case, although J_k vanishes for $k \to 0$, the overall scaling behaviour remains the same as in the free b.c. case.

Finally, we wish to mention that the modal analysis can help to shed some light on a futher open problem: the determination of the temperature profile. We have seen that different models (such as harmonic and FPU chains) are characterized by energy equipartion even out of equilibrium. This is true even though they exhibit very different spatial profiles. It is quite natural to conjecture that this is caused by different phase correlations among the various modes, but working out a detailed explanation appears not to be a trivial task.

VI. THE 2D FPU

The presence of an energy threshold for the relaxation dynamics has been observed also in 2d lattice models of anharmonically coupled oscillators. For instance, in [40] the authors investigated a square–lattice of oscillators coupled by a Lennard–Jones 6/12 potential

$$V(r) = A\left[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}\right] \tag{22}$$

where $r = |\vec{r}|$ is the modulus of the distance vector $\vec{r}$ between nearest-neighbor oscillators. At energy den-

sity $e_c \approx 0.3$ they observed a crossover from a high–temperature regime of strong chaos to a low–temperature weakly chaotic regime. Specifically, above e_c wave-packet excitations of low wave-number harmonic modes were found to relax very rapidly to a thermalized state, characterized by the equipartition of the energy among the Fourier modes. Below e_c the weakly chaotic relaxation dynamics exhibited a slowing-down of the energy equipartition, and the evolution appeared increasingly far from ergodic, while decreasing the energy density. In this regime, fluctuations of particles around their equilibrium positions are quite small, so that potential (22) can be very well approximated by its Taylor series expansion

$$V(r) = \frac{1}{2}\omega r^2 + \frac{1}{3}\alpha r^3 + \frac{1}{4}\beta r^4 + \cdots \qquad (23)$$

where the parameters ω, α and β can be expressed in terms of A and σ. This indicates that a very similar scenario is expected to hold also in the 2d FPU model, whose potential has the form reported on the r.h.s. of (23).

More recently, the FPU model has been investigated on a triangular 2d lattice [41]. It has been observed that the slowing-down of energy equipartition for sufficienty small values of e is definitely less a dramatic effect than in the square lattice case. In particular, while increasing the size of the system there is evidence that in the triangular lattice a threshold value is better identified by the total energy E , rather than by the energy density e. This implies that the effects of weak chaos should vanish in the thermodynamic limit much more rapidly than in the square–lattice case. Nonetheless, all of these results can be interpreted consistently by considering that a typical feature of lattices of anharmonic oscillators is the appearance of long time scales for relaxation of excitations towards a thermalized state (equilibrium) as soon as the energy is sufficiently small. Accordingly, this fact is expected to have some important consequences on the heat transport also in 2d lattices. Actually, this problem has been investigated for the FPU and the Lennard-Jones models in [42]. Numerical simulations performed for lattice size N up to $\mathcal{O}(10^2)$ indicate that in the strong chaotic regime the thermal conductivity diverges logarithmically with the system size, $\kappa(N) \sim \ln N$. This is consistent with the theoretical prediction of the mode–coupling theory, which is obtained by estimating the average value of the heat–flux time correlation function at thermal equilibrium [5]. Conversely, in the weak chaotic regime the thermal conductivity seems to diverge according to a power-law, $\kappa \sim N^\eta$. The exponent η increases while decreasing e below e_c and it is expected to approach unit for vanishing e, since in this limit the harmonic lattice is recovered. In analogy with what observed in 1d, it seems reasonable to assume that also in 2d one should eventually recover the logarithmic divergence also in the weak chaotic regime for sufficiently large system size and sufficiently long integration time. On the other hand, the practical difficulty of performing more extended numerical simulations prevents the possibility of verifying this conjecture. Moreover, it should be mentioned that there are also conflicting results indicating that the 2d scenario is still quite far from being fully understood. For instance, further numerical simulations performed for the 2d FPU square-lattice were found to be compatible with a power-law divergence of the heat conductivity, with an exponent $\alpha \approx 0.22$ [35]. In these simulations the authors used larger system sizes than those used in [42]. Accordingly, their results should be considered more reliable for what the dependence of κ on N is concerned, although noone among the available theoretical arguments supports such a prediction. It should be also noted that in [35] the measurement of $\kappa(N)$ was obtained by non-equilibrium simulations with heat baths at relatively moderate temperatures with respect to those employed in [42]. Although the values of the temperature chosen in [35] are still in the range of strong chaos, they are not far from e_c and one cannot exclude that the observed power–law behavior could be just an artifact of finite–size corrections already effective at temperatures too close to the so–called equipartition threshold.

VII. CONCLUSIONS

In spite of the many efforts made in the 50 years that separate us from the first numerical simulation performed by Fermi, Pasta and Ulam, one cannot yet onclude that heat conduction is fully understood. We discussed how the simple, apparently harmless, FPU model may serve to illustrate how both weakly chaotic dynamics and reduced dimensionality affect the validity of macroscopic transport laws.

Instances of open problems are the shape of the temperature profile which depends on boundary conditions and coexist with energy equipartion like in equilibrium, when temperature is constant across the system. The effective coupling between thermal baths and (low- and high-frequency) Fourier modes is a related problem, whose solution might help in identifying those boundary conditions which can minimize the contact thermal resistance. A deeper understanding of these issues in toy models like FPU may be illuminating to describe energy transport in "small systems" like single–molecules or nanostructured materials.

The dependence of the time (and, correspondingly, the length) to reach the asymptotic scaling regime on the energy density at low temperatures represents another open problem. The results here reported indicate that the time needed for a nonlinear behaviour of the hydrodynamic modes to set in increases as an inverse power of the energy density. The scaling behaviour is compatible with that exhibited by the times required for the chaotization of generic trajectories, although it follows from the analysis of completely different dynamical processes. Accordingly, we are led to conjecture that in the thermo-

dynamic limit the evolution is controlled by a single time scale. Last but not least, the scenario in 2d FPU lattices is even more unclear, the nature of the leading behaviour being still questioned.

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$$J \;=\; \frac{a}{2}\sum_n (\dot{x}_{n+1}+\dot{x}_n)\,F_n \;-\; bv_0\langle\sum_n F_n\rangle \quad ,$$

with v_0 being the center–of–mass velocity. This is necessary to ensure that the autocorrelation of J appearing in the Green-Kubo formula vanishes for large times.
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